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14. ABSTRACT

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One solution to this problem is symmetry-adapted perturbation theory based on DFT description of monomers

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One solution to this problem is symmetry-adapted perturbation theory based on DFT description of monomers [SAPT(DFT)]. In applications to energetic materials, SAPT(DFT) predicted the correct crystal structure of RDX (1,3,5¬trinitroperhydro-1,3,5-triazine). Recently, the complete PES of FOX-7 (1,1-diamino-2,2-dinitroethene) dimer was obtained using SAPT(DFT). Preliminary molecular dynamics simulations of the FOX-7 crystal show an improved agreement with experiment compared to literature results. A recently developed nearly-linear scaling implementation of the SAPT(DFT) dispersion energy has been applied to interactions of energetic molecules. When the development of linear-scaling SAPT(DFT) is finished, accurate studies of energetic molecules significantly larger than RDX and of other important systems (including biomolecules), containing in excess of one hundred atoms, will be possible. Another approach which can be applied to such systems is the dispersion-less density functional (dlDF) method developed in our group which reproduces interaction energies with the dispersion component removed. The dispersion energy is then computed from an asymptotic function fitted to SAPT(DFT) dispersion energies of a training set, resulting in a method denoted as dlDF+D. Cross sections of the PES of the HMX (octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocane) dimer calculated using dlDF+D are presented.

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Dispersion Interactions in Calculations of Properties of Energetic Materials

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Abstract

Until recently, first-principles calculations of potential energy surfaces (PES) were restricted to intermolecular interactions involving molecules containing just several atoms. On one hand, this was due to the high cost of wave-function-based electronic structure methods and, on the other hand, to the failure of the density functional theory (DFT) approaches to reproduce the dispersion part of intermolecular interactions.

One solution to this problem is symmetry-adapted perturbation theory based on DFT description of monomers [SAPT(DFT)]. In applications to energetic materials, SAPT(DFT) predicted the correct crystal structure of RDX (1,3,5¬trinitroperhydro-1,3,5-triazine). Recently, the complete PES of FOX-7 (1,1-diamino-2,2-dinitroethene) dimer was obtained using SAPT(DFT). Preliminary molecular dynamics simulations of the FOX-7 crystal show an improved agreement with experiment compared to literature results. A recently developed nearly-linear scaling implementation of the SAPT(DFT) dispersion energy has been applied to interactions of energetic molecules. When the development of linear-scaling SAPT(DFT) is finished, accurate studies of energetic molecules significantly larger than RDX and of other important systems (including biomolecules), containing in excess of one hundred atoms, will be possible.

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1. Introduction

Energetic materials are important to the national defense, and the study of their bulk properties represents one of the most active fields of the material sciences. Some of the obvious disadvantages of experimental research in this area are the relatively high risk involved and associated costs, especially when synthesizing and testing new materials of yet unknown properties. Therefore, a reliable theoretical prediction of the crystal structure and other physicochemical properties of such compounds is highly desirable. The most important prerequisite for achieving this goal is the availability of an intermolecular potential (force field) representing the interaction energy of a pair of molecules as a function of their separation and orientation. One possible way to develop such potentials is to fit their functional form (including a number of adjustable parameters) so as to reproduce as closely as possible certain experimental data. The most serious drawback of empirical force fields is their uncertain predictive power. Since such fields only contain information about the pertinent system under the conditions corresponding to the data used in the fitting, these potentials often fail when applied to significantly different conditions or to properties not related to those data. On the other hand, *ab initio* potentials are obtained from first-principles quantum mechanical calculations and can be, formally, as accurate as desired, provided that a sufficiently large basis set and a high level of theory, especially an appropriate description of the electron correlation, are used. Wave-function-based methods, such as the coupled cluster theory or symmetry-adapted perturbation theory (SAPT), are quite demanding computationally, and their cost scales too steeply with the system size to be applicable to accurate calculations of molecules larger than about a dozen of atoms. Density functional theory (DFT), while significantly less expensive, poorly describes long-range dynamic correlation effects, and thus the dispersion interaction, which is often the predominant effect in compounds forming molecular crystals. Because of this dilemma, a successful first-principles simulation of energetic materials was not possible as recently as a decade ago. The situation changed with an advent of new methods combining the advantages of various distinct theories. The symmetry-adapted perturbation theory with the density-functional theory description of monomers[1–7], abbreviated as SAPT(DFT) or DFT-SAPT, is similar to the regular SAPT approach, but represents the monomers using the Kohn-Sham DFT approach[8] instead of the much more expensive coupled cluster theory. The crucial dispersion interaction is calculated from the so-called frequency-dependent density susceptibilities (FDDS) (i.e., polarization propagators) of the monomers[4,5], which in turn can be obtained from a coupled Kohn-Sham (time-dependent DFT) calculation. A big advantage of the SAPT(DFT) approach is the fact that the full dimer calculation is entirely avoided and the once-computed FDDS's of the monomers can be used for any dimer configuration, provided that the monomers are rigid. The density-fitting technique[9] has been implemented in this method[10–12] and has resulted in an additional improvement of the efficiency. The SAPT(DFT) approach was applied to such computationally demanding problems as the complete PES of the benzene dimer[13] and selected configurations of the pyrene dimer[14], the latter containing as many as 52 atoms. In the field of energetic materials, SAPT(DFT) has been very successful[15–17] in predicting the correct crystal structure of RDX (1,3,5-trinitroperhydro-1,3,5-triazine), with the dimer of RDX containing 42 atoms. We also calculated the complete PES of the FOX-7 (1,1-diamino-2,2-dinitroethene) dimer and here we report some initial results of the simulations for the FOX-7 crystal.

The application range of SAPT(DFT) can be extended to still larger dimers, of the size in excess of a hundred of atoms, by the near-linear scaling version, L-SAPT(DFT). In this approach, one divides the set of atoms in each monomer into a “far-region” and a “near-region” subsets. The far-region atoms are those whose distance from every atom in the other monomer is larger than a certain cutoff value, R_{cut}. Obviously, for very large molecules most atoms belong to the far region. Since the dimer interaction can be represented as a sum of interactions between disjoint regions of both monomers, only a small fraction of the total calculation (between near-region atoms of both monomers) has to be performed using the regular SAPT(DFT) expressions, while the rest can be sufficiently accurately evaluated from simple asymptotic formulas. The results of L-SAPT(DFT) calculations have already been reported for the electrostatic energy[18] and the strategy described above has recently been implemented for the dispersion energy. Our initial results for the latter component are presented below.

Recently, our group introduced[19] another new hybrid method for calculations of interaction energies with a large dispersion component. The idea of this method is based on the observation that DFT should be able to quite accurately predict all the components of the interaction energies but the dispersion energy. Consequently, a “dispersionless” density functional (dlDF) has been optimized[19] to reproduce the dispersionless interaction energies, i.e., the interaction energies with the dispersion components subtracted, for a training set containing nine common dimers at various intermonomer separations. The interaction energies were obtained using the coupled cluster method with single, double, and noniterated triple excitations [CCSD(T)], while the dispersion energies were represented by the sum of the second-order dispersion and exchange dispersion energies, $E^{(2)}_{\text{disp}} + E^{(2)}_{\text{exch-disp}}$, calculated with SAPT(DFT). The interaction energies produced by dlDF calculations must, of course, be supplemented with dispersion energies obtained by some other method, forming a hybrid approach known as dlDFT+D. Up to some dimer size, one can use the dispersion energies computed using SAPT(DFT). For larger systems, the authors of Reference 19 developed a simple damped asymptotic dispersion function, in the form of a sum of pair (atom-atom) contributions. Its parameters were optimized to reproduce the sum $E^{(2)}_{\text{disp}} + E^{(2)}_{\text{exch-disp}}$ on a training set. The dispersion function was significantly improved in Reference 20 by introducing different parameter values for hydrogen atoms, depending on their connectivity, and by enlarging the training set. This form of the dlDFT+D approach was used in the present work.

2. FOX-7 Calculations

The SAPT(DFT) method was recently used to calculate about 1,300 points of the FOX-7 dimer PES. A pair potential based on Coulomb terms describing the interaction between partial charges on atoms plus Buckingham-type exp-6 terms was obtained. The partial charges were determined by fitting to *ab initio* molecular multipole moments of the monomer (through l=6). The remaining parameters were fitted to the SAPT(DFT) interaction energies directly. Here we present (see Table 1), for the first time, results of a NsT (constant number of molecules, stress, and temperature) simulation of the crystal lattice parameters, based on the new potential, compared to the semi-empirical potential of Sorescu, et al.[21]. Except for the lattice dimension *a*, the SAPT(DFT) potential clearly improves the agreement with experimental data and the error of the unit cell volume is reduced by a factor of 1.7. The work on FOX-7 is in progress. In particular, calculating new PES points in some critical regions is still an option, which would likely further improve the agreement with experiment.

Table 1. Results of the NsT simulation of the FOX-7 crystal lattice at 300K. The unit cell parameters are in angstroms (*a*, *b*, *c*) and degrees (*α*, *β*, *γ*), the volume in Å^3.

method	a	b	c	α	β	γ	volume (%error)
Experiment [22]	6.93	6.62	11.31	90.00	90.06	90.00	519
Ref. [21]	6.93	6.86	11.60	89.99	89.79	89.98	551 (6.2)
SAPT(DFT)	6.79	6.54	11.25	89.99	90.02	89.98	500 (3.7)

3. HMX Dimer Calculations

The HMX (octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocane) molecule is an eight-membered analogue of the six-membered RDX ring and its dimer has 56 atoms. HMX exists in four different polymorphic forms, labeled α through δ. The form stable at ambient conditions, *β*-HMX, crystallizes in the monoclinic space group $P2_1/c$. It is the only crystal structure of HMX containing molecules in the C_i-symmetry conformation (the three other forms contain C_2-symmetric molecules). The bulk properties of HMX crystals were the subject of numerous atomistic simulation papers[23–38]. However, to our knowledge, there is no accurate study of the dimer in the literature. We performed such a study applying the dlDF+D method. First, we used the simple HMX pair potential developed in Reference 24 to perform a quick scan of the PES. The *β*-HMX monomer geometry was retrieved from the Cambridge Structural Database (code OCHTET12). It was kept frozen throughout all the calculations, i.e., only the rigid-monomer dimer configurations were studied. We calculated the dimer interaction energies on the six-dimensional grid constructed by taking all the center-of-mass (COM) distances *R* from 5 to 7.25 Å with a step of 0.25 Å and all the possible relative Euler angles with a step of 10°. The geometry corresponding to the lowest energy was subsequently refined in several steps by forming denser and denser grids around the current minimum. The obtained minimum energy structure (interaction energy equal to −5.86 kcal/mol) is presented in Figure 1. It has the COM distance of 5.42 Å and both molecules are almost exactly parallel (with a small deviation of 4° caused probably by the fact that the monomer of Reference 24 does not have the exact C_i symmetry).

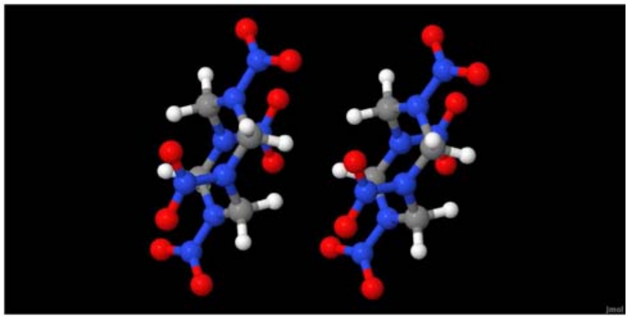


Figure 1. Minimum energy geometry of the HMX dimer

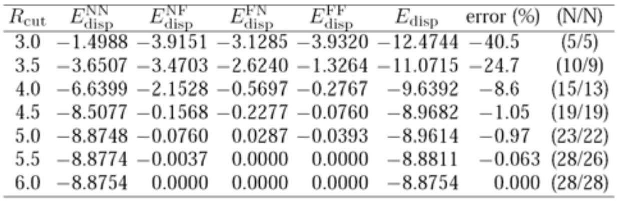
In the next step, we used the dlDFT+D method and the correlation-consistent augmented double-zeta Dunning basis set (aug-cc-pVDZ, 1064 basis functions)[39] to obtain a cross section of the HMX dimer PES, containing the structure of Figure 1 and thirteen other structures with the same relative orientation and with *R* ranging from 4.75 to 8 Å. The summary of the results is presented in Table 2. Qualitatively, the shape of both interaction potentials, empirical and dlDF+D, along this cross section is similar. However, the dlDFT+D calculation predicts a significantly deeper minimum (−7.00 vs. −5.86 kcal/mol) at a slightly shorter COM distance (5.30 vs. 5.42 Å). The interaction is strongly dominated by the dispersion energy, which is (at the minimum distance) 2.5 times larger in absolute value than the sum of the remaining components.

Table 2. HMX dimer interaction energies E_{int} (in kcal/mol) for the orientation of the Sewell's potential[24] global minimum as functions of the center-of-mass distance between the monomers, *R* (in angstroms). E_{rep} and E_{elec} stand for the repulsion and electrostatic energy terms in the potential of Reference 24 and E_{disp} for the dispersion energy calculated with either method.

	dlDFT+D method			potential of Ref. [24]		
R	dlDFT	E_{disp}	E_{int}	$E_{\mathrm{rep}} + E_{\mathrm{elec}}$	E_{disp}	E_{int}
4.75	24.1528	−24.7671	−0.6143	29.0331	−24.5247	4.5084
5.00	11.9230	−17.4288	−5.5058	14.3095	−17.2939	−2.9844
5.20	6.4220	−13.2496	−6.8276	7.9889	−13.2431	−5.2543
5.25	5.4408	−12.3852	−6.9444	6.8905	−12.4098	−5.5193
5.30	4.5832	−11.5824	−6.9993	5.9382	−11.6369	−5.6987
5.35	3.8384	−10.8367	−6.9983	5.1133	−10.9194	−5.8061
5.42	2.9629	−9.8804	−6.9176	4.1417	−9.9998	−5.8581
5.50	2.1521	−8.9008	−6.7487	3.2492	−9.0575	−5.8083
5.70	0.7586	−6.8945	−6.1359	1.7567	−7.1227	−5.3660
6.00	−0.2075	−4.7742	−4.9817	0.6843	−5.0573	−4.3729
6.50	−0.6952	−2.6995	−3.3947	0.1356	−2.9839	−2.8482
7.00	−0.7372	−1.6057	−2.3429	0.0254	−1.8442	−1.8187
7.50	−0.6655	−0.9993	−1.6648	0.0044	−1.1850	−1.1806
8.00	−0.5764	−0.6467	−1.2231	0.0005	−0.7869	−0.7864

Table 3 shows results of the application of the new, near-linear scaling dispersion code of the SAPT(DFT) method to one of the configurations from Table 2 (R=5.42 Å). The basis set of Sadlej[40] was used, containing 552 basis functions per monomer. The calculation with the largest cutoff distance, R_{cut}=6.0 Å, assigns all the atoms to the near region, which results in the application of the regular SAPT(DFT) algorithm and yields the exact (within this particular basis set) value of the dispersion energy, E_{disp}=−8.88 kcal/mol. This benchmark result can be compared with the value from the damped asymptotic dispersion function of the dlDFT+D method, equal to −9.88 kcal/mol (11% of error). In fact, the true discrepancy is somewhat larger since the former value does not include $E^{(2)}_{\text{exch-disp}}$, which is positive. Reducing the cutoff distance introduces a gradually increasing error of the L-SAPT(DFT) dispersion energy, but up to R_{cut}=4 Å, where half of all the atoms are in the far region, L-SAPT(DFT) predicts the dispersion energy more accurately than the current version[20] of the dlDFT+D dispersion fit. It should be noted that this particular system represents a rather unfavorable case for a L-SAPT(DFT) calculation. As seen in Figure 1, both molecules are stacked in a near-sandwich configuration, where the near region necessarily extends to a significant portion of both molecules. With the current code, a single calculation of the HMX dimer interaction energy requires between 2 and 3 CPU-days with either dlDFT+D or L-SAPT(DFT) on the MJM linux cluster (3.0 GHz Intel Woodcrest processors) at US Army Research Laboratory (ARL).

Table 3. L-SAPT(DFT) HMX dimer dispersion energy E_{disp} and its four parts (in kcal/mol) for the geometry of the Sewell's potential[24] global minimum as a function of the cutoff distance, R_{cut} (in angstroms). $E^{\text{XX}}_{\text{disp}}$ denotes the contribution from the near region (X=N) or far region (X=F) of the monomers. $E^{\text{NN}}_{\text{disp}}$ was calculated from the exact SAPT(DFT) formulas and the other three contributions from asymptotic formulas. (N/N) stands for the number of near-region atoms in both monomers.



R_{cut}	$E^{\text{NN}}_{\text{disp}}$	$E^{\text{NF}}_{\text{disp}}$	$E^{\text{FN}}_{\text{disp}}$	$E^{\text{FF}}_{\text{disp}}$	E_{disp}	error (%)	(N/N)
3.0	−1.4988	−3.9151	−3.1285	−3.9320	−12.4744	−40.5	(5/5)
3.5	−3.6507	−3.4703	−2.6240	−1.3264	−11.0715	−24.7	(10/9)
4.0	−6.6399	−2.1528	−0.5697	−0.2767	−9.6392	−8.6	(15/13)
4.5	−8.5077	−0.1568	−0.2277	−0.0760	−8.9682	−1.05	(19/19)
5.0	−8.8748	−0.0760	0.0287	−0.0393	−8.9614	−0.97	(23/22)
5.5	−8.8774	−0.0037	0.0000	0.0000	−8.8811	−0.063	(28/26)
6.0	−8.8754	0.0000	0.0000	0.0000	−8.8754	0.000	(28/28)

4. Conclusions

The recent progress in developing computationally efficient first-principles methods of studying molecular interactions, especially in dealing with the dispersion energy treatment, has made possible a systematic study of dimers where first-principles calculations were prohibitively time-consuming just a few years ago. In particular, our pilot calculations for the HMX dimer (56 atoms) show that obtaining the complete PES for this important energetic material is now feasible. Assuming that a similar number of PES points as that for FOX-7 are required, the complete project will consume around 100K CPU-hours.

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